ANL/NSE-C2017-17215

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# Joint Development of SAS4A Code in Application to Oxide-fueled LFR Severe Accident Analysis

*Final CRADA Report*

**Nuclear Science and Engineering**

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# Joint Development of SAS4A Code in Application to Oxide-fueled LFR Severe Accident Analysis

*Final CRADA Report*

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**Non Proprietary**

# Final CRADA Report

For the Office of Scientific and Technical Information (OSTI)

**CRADA Number:** A17215
**CRADA Title:** Joint Development of SAS4A Code in Application to Oxide-fueled LFR Severe Accident Analysis
**CRADA Start Date** 4/19/2018 – **End Date** 4/18/2020

**DOE Program or Other Government Support**
**Program office:** DOE, Office of Technology Transfer

## Participant

**Participant name:** Westinghouse Electric Company, LLC
**Complete address:** 1000 Westinghouse Drive, Cranberry Township, PA 16066-5528

## Argonne National Laboratory

Argonne PI(s): Tanju Sofu

## Funding Table

To add rows, right-click in bottom row and select “Insert” “rows above”.

| | Planned Funding | Actual Funding | In-Kind |
|---|---|---|---|
| Government | $390,000 | $390,000 | |
| Westinghouse Electric Company, LLC | $410,000 | $10,000 | $400,000 |
| **Total** | **$800,000** | **$400,000** | **$400,000** |

## Nature of Work

**Describe the research (summary of Scope of Work and principal objectives of the CRADA):**
The scope of this project was to pursue specific SAS4A liquid-metal cooled reactor (LMR) safety analysis software extensions to simulate postulated accidents with fuel failures for oxide-fueled Lead-cooled Fast Reactors (LFRs). Since most U.S. LMR experience is on sodium-cooled fast reactor options based on past testing and operation experience with EBR-II and FFTF, the DOE’s legacy fast reactor safety analysis capabilities were focused on metal-fueled pool-type concepts with sodium coolant. In recent years, Westinghouse Electric Company (WEC) has decided to pursue an LFR design as one of their next generation nuclear technology options because of its favorable safety and economics attributes. Oxide fuel is considered among other fuel options due to previous WEC experience with this fuel form. Development of this new technology requires the availability of adequately accurate computational tools, some of which can be adapted from versions of similar software used for analysis of other LMRs. Although Argonne National Laboratory’s (ANL) SAS4A/SASSYS-1 safety analysis software suite (shortened as SAS4A code hereafter for brevity) has the basic capabilities to model LFR system designs, the SAS4A code modules used in the analysis of accidents with fuel/cladding failures lack appropriate models for the unique phenomena that govern as-irradiated oxide-fuel damage mechanisms in lead coolant. Therefore, the objective of this project was to extend the capabilities of SAS4A with mechanistic oxide-fuel failure models in lead coolant for margin to failure assessments, analysis of failure modes, location and timing of failures under different accident scenarios consistent with the whole-plant dynamic response including the reactivity feedback, and assessment of the potential for fuel damage propagation due to potential fission gas jet and fuel-fragment/molten fuel impingement to neighboring fuel pins in an assembly. This report provides mainly a summary of Argonne’s technical contributions in the joint project, but the reports and publications by the Participant team are included as references at the end of the report.

**DOE mission area(s):**
Energy and Environmental Science and Technology

**Conclusions drawn from this CRADA; include any major accomplishments:**

SAS4A LFR Model Used to Support the Development

To support the project goals and to serve as a test bed for newly developed code features, a SAS4A model of an LFR design (CLFR) selected by Westinghouse, and representative of the one being pursued by the company, was first developed. All the design information on CLFR used for the model was provided by Westinghouse, along with the results of core neutronics analysis required for a SAS4A model. Since the design used for the assessments below was for demonstration of the SAS4A code capabilities, the results presented in this report are not expected to be representative of the final Westinghouse LFR design.

The SAS4A model for CLFR consists of three major parts: The core model, primary loop model, and reactor control system. The core model consists of five channels: Channels 1 through 3 represent average fuel assemblies in the inner, middle, and outer core regions, respectively. Channel 4 simulates all non-fuel assemblies, including reflector, shield, and control. Channel 5 is the peak power assembly to calculate peak coolant, cladding, and fuel temperatures in the core. Two versions of the SAS4A core model were developed: one for the beginning-of-fuel-cycle (BOC) conditions, and the other for the end-of-cycle (EOC) conditions. The CLFR core model includes modeling of the reactivity feedbacks due to fuel Doppler, fuel and cladding axial expansion, coolant density, core radial expansion, and control rod driveline expansion. The core model also incorporates the newly developed oxide fuel deformation model in SAS4A.

The primary loop model of CLFR represents all primary coolant inside the reactor vessel. The modeled primary loop components include the reactor core, primary coolant pumps, primary heat exchangers, and corresponding cold and hot coolant pools. The primary loop model also includes RVACS system to remove heat from outside the reactor vessel. Since no design information is currently available for CLFR beyond the primary loop, the SAS4A model doesn't include any systems and components for the energy conversion part of the plant. Instead, the boundary conditions are applied to the primary heat exchangers.

SAS4A control module is used to simulate action of the CLFR passive reactor trip system. The input to this module was developed to simulate insertion of the control rods into the core (with -5$ worth) once the hot pool temperature reaches a certain level (700 °C). However, this action was intentionally disabled to simulate much less likely unprotected (un-scrammed) transients described below.

To demonstrate the capabilities of the SAS4A model, two sample transients were considered. Both transients were modeled as "unprotected" transients meaning that the normal reactor protection is also postulated to fail in the accident. Thus, the reactor power is controlled by internal reactivity feedbacks only.

The unprotected transient overpower (UTOP) at BOC conditions simulates a malfunction of a control rod by introducing positive external reactivity. The external reactivity addition is compensated by negative reactivity feedbacks, dominated by fuel Doppler and core axial expansion. These negative reactivity feedbacks provide enough reactivity to preclude fuel melting during this accident, even as power is calculated to reach about 200% level from the control rod malfunction. The maximum cladding temperature is calculated to reach a peak value of 1000 °C before stabilizing at a lower level. Since the accident is simulated for BOC conditions with relatively fresh fuel and due to relatively short duration of the transient, the cladding cumulative damage function (CDF) is calculated not to exceed a value of $10^{-5}$ in this accident.

The unprotected station blackout (USBO) transient at EOC conditions simulates a sudden loss of power for all primary and feedwater pumps. The primary pumps are assumed to have no inertia and the pump head drops to zero immediately after the start of the transient. Similar to the UTOP transient, an unprotected transient is simulated under an assumption of failure of the reactor protection system. Reduction in primary flow rate increases temperatures in the core, which introduces negative reactivity to reduce the core power. In this case, the reactivity feedback is dominated by the core radial expansion. The transient is analyzed for the short-term (about 15 minutes) and the long-term (1 day) behavior of the reactor during this accident. In the short term, the peak cladding temperature increases to about 1000 °C, while fuel melting is still avoided. In the long term, the heat removal is provided by RVACS whose heat removal capacity is calculated to exceed decay heat production in the core at about 4 hours into the transient, where the peak pool temperatures of 880°C are calculated. After that, the entire system slowly cools down, reaching pool temperatures of 770°C by the end of transient simulation.

The cladding CDF is calculated to increase to $10^{-3}$ by 10 hours into the transient and does not increase afterwards.

Overall, both transients show safe reactor response even under these severe (and very low frequency) transients with unprotected (un-scrammed) conditions. The results of the transients are used further in this project for more detailed prediction of cladding failure. Since only two sample transients were analyzed in this work, more transients need to be investigated in the future to complete the safety analysis of CLFR and conclude whether the reactor meets its safety criteria.

Development of New SAS4A Modules for Mixed-Oxide (MOX) Fuel in Lead Coolant

The goal of this part of the effort was to improve and validate the MOX fuel and cladding models of SAS4A to enhance fuel failure predictions particularly for LFRs. Activities were focused on (1) improving the physical models of DEFORM-4 MOX fuel performance module of SAS4A, (2) Implementing 15-15Ti cladding mechanical and creep rupture properties, (3) performing validation exercises for the new models of DEFORM-4 using the available pre-transient and transient databases, (4) implementing a stochastic clad failure propagation model specifically for LFRs, and (5) completing the software quality assurance procedure to integrate new models into the release version of SAS4A code and its manual.

DEFORM-4 Module MOX Fuel Performance Modeling Improvements:

Fission Gas Behavior: The new fission gas behavior module tracks fission gas in fuel matrix, intragranular gas bubbles, and intergranular gas bubbles, separately. During pre-transient simulation, the intragranular gas is partitioned to dissolved gas in matrix and gas in intragranular gas bubbles using relations for the rate of gas trapping by the bubbles and rate of gas dissolution from the bubbles. During the transients, intragranular gas bubble coarsening, their movement under the temperature gradient and deposition at the grain boundaries are modeled using a rate theory model. The lenticular bubbles at intergranular sites are modeled as an intergranular gas bubble network. When the concentration of the intergranular gas bubbles exceeds the threshold value, tunnels form at the intergranular sites and gas release to the free volume of the fuel pin starts for the corresponding node. The role of fuel chemistry evolution on the fission gas behavior is modeled by modifying the gas diffusivity as a function of the Oxygen-to-Metal ratio of the fuel. The inwards fuel swelling behavior that was observed for the irradiated annular MOX fuels is also included in the new models so that the fuel can swell inwards during normal operation as well as during transients. It was found that this enhancement improved the predictions of the validation test cases significantly.

Fuel Chemistry: Fuel chemistry evolution directly affects thermal, mechanical and fission gas behavior of the Mixed Oxide (MOX) fuel. Volatile behavior of Cesium is modeled by a rate equation such that fuel swelling due to cesium decreases at elevated temperatures. Oxygen-to-Metal ratio (O/M) of the MOX fuel is tracked as a function of burnup. The radial redistribution of oxygen under the temperature gradient driving force is also computed using a diffusion model for each axial location. The formation of CsMoO4 Joint-Oxide Gain (JOG) at the fuel outer surface and its effect on fuel swelling and gap conductance is modeled as a function of O/M evolution, burnup, temperature and Cesium concentration. It is also assumed that JOG formation rate is proportional to the fission gas release at the corresponding node. Cladding inner corrosion due to intergranular attack of Cs, I, Te is modeled by a rate theory equation as a function temperature, O/M and burnup. Finally, Pu radial redistribution is modeled using a diffusion model based on thermo-transport theory. Pu redistribution could affect the fuel melting temperature. Currently, this effect has not been coupled with thermal models.

Thermal Behavior: The thermal conductivity and gap conductance models have been updated in this study. Lucuta's thermal conductivity model which is based on JOYO MOX fuel database and which accounts for O/M, burnup, porosity dependencies explicitly, has been adopted in this study. To compute the gap conductance between the cracked fuel surface and the cladding, it is assumed that the heat passes through JOG layer and gas layer. The porosity in JOG is conservatively assumed to be 50 % while computing the thermal conductivity of the JOG layer. The conductance through the gas layer is computed using DEFORM-4's modified Ross-Stoute model. Then the effective thermal resistance between the fuel surface and clad inner surface is used to compute the temperatures.

15-15Ti Cladding Properties: The properties needed for the fuel performance have been integrated into SAS4A. Irradiation induced void swelling, irradiation creep, thermal creep, and thermal creep rupture correlations

are added. The assessment of the creep rupture margin of the cladding is now computed by a Cumulative Damage Fraction type model. This new feature allows DEFORM-4 to compute the clad failures during transients that are not rapid enough to cause clad failure due to overloading. In addition, clad outer corrosion due to interaction between lead coolant and stainless steel cladding can now be set as a SAS4A input.

Fuel Pin Mechanics: New models have been introduced for simulating the fuel dimensional changes, fuel cracking, fuel hot pressing, and fuel clad mechanical interaction. Given the strain components of the fuel pellet and cladding, the interfacial pressure is computed iteratively by a predictor corrector algorithm. The new mechanics model is capable of predicting the mechanical behavior below yield stress and creep rupture of the cladding during slow UTOP as well as the behavior above the yield stress and clad failure due to overloading during rapid UTOP scenarios.

Stochastic Clad Damage Propagation Model: A stochastic clad damage propagation model has been developed and implemented into SAS4A as a sidebar calculation applicable to LFR conditions. The goal is to predict the clad failure by random sampling and quantify the decrease in clad failure margin for the neighbor fuel pins due to post-failure release of fission gas and fuel particles (a model that has been developed in this project). Based on the literature review, it is assumed that a clad failure can only affect the two of the neighbor fuel pins that belong to the same subchannel where failure took place. Probability of the clad failure of individual fuel pins is characterized by a normal distribution which is given as a function of logarithm of CDF (clad life fraction). Every SAS4A fuel channel is represented by the average fuel pin, which corresponds to the default fuel pin in SAS4A per channel, and the fuel pins adjacent to the failed fuel pins that are thermally affected by the fission gas and fuel mixture jet. Latter pins are called neighbor fuel pins. Given the CDF, the probability of failure of all fuel pins are summed up. When this sum is greater than 1, a random sampling procedure is applied to decide which fuel pin failed. If the failed pin is an average fuel pin, two adjacent fuel pins belonging to the same subchannel with the failure location are assigned as neighbor fuel pins. At this moment, fission gas and fuel mixture ejection model is activated to compute the clad temperature increase and corresponding increase in CDF in neighbor fuel pins. If the failed pin is a neighbor fuel pin, no new neighbor is generated indicating that the failure propagation should be attested by the corresponding subchannel. Instead, the remaining neighbor pin that was previously paired with the failed neighbor pin gets degraded by the fission gas and fuel mixture jet. The resulting model has been applied to CLFR design for assessment of total number of failed pins in selected transients.

Validation of the New MOX Fuel Performance Models:

The extended DEFORM-4 oxide fuel models of SAS4A have been benchmarked using the measured data for the pre-transient fission gas behavior, separate effect transient fission gas behavior during rapid heating conditions, CABRI slow TOP and CABRI Rapid TOP experiments. The measured fission gas release, retained fission gas in fuel, clad failure time and location and fuel melt boundary were compared with the SAS4A predictions. The benchmark sets have a burnup range between 1 at% to 23 at% operated at PHENIX, JOYO and PFR. Both solid and annular fuel configurations are included.

The pre-transient part of the extended MOX fuel performance models has been benchmarked using the results of six tests. RIG1 and RIG2 solid fuel pins, SCARABIX and VIGGEN-4 annular fuel pins were irradiated in PHENIX. MK-2 solid fuel pin and LVD annular fuel pin were irradiated in JOYO and PFR, respectively. Pre-transient benchmarks showed that the code can predict the axial distribution of the retained fission gas, burnup variation of the cumulative fission gas release and fuel pin mechanical behavior satisfactorily.

Separate effect tests conducted at Hanford Engineering and Development Laboratory (HEDL) to describe the response of rapid heating of irradiated MOX fuel have been utilized to benchmark transient fission gas model of new DEFORM-4. The MOX fuel samples were irradiated at EBR-II. The test fuel samples were placed inside a capsule. During the experiment, the capsule was electrically heated, and temperature and pressure were recorded. Using the measured fission gas pressure, transient fission gas release of MOX fuel samples was derived from the experiments. A large amount of fission gas release was measured in the experiment when the sample temperature rises to near fuel melting temperature in eight seconds. It was found that the new transient intragranular gas behavior module that accounts for the bubble coarsening and movement towards the grain boundaries during the transient can predict the transient fission gas release behavior with $\pm$10% error.

Slow TOP test results performed under CABRI-2 experimental program with 15-15Ti cladding have been used to benchmark the extended DEFORM-4 models. Two of the tests adopted has VIGGEN-4 fuel pins and three of

the tests used SCARABIX fuel pins. During the tests, the power ramped from typical operating conditions to 80 kW/m to 125 kW/m peak linear heat rate. Test pins were subjected to excessive fuel melting and some pins experienced cladding failure. The benchmark demonstrated that the code can well predict 15-15Ti clad failure time and location, axial distribution of the molten fuel fraction and transient fission gas release behavior.

Software Quality Assurance of the New MOX Fuel Performance Models

Software quality assurance procedure for the new MOX fuel performance models includes setting and documenting the software requirements specifications, software design description, software test plan, SQA compliant code implementation, and code manual integration. Verification unit tests were developed to test every pieces of the physics module that has been implemented, the input and the output. As a result of the SQA process, the developmental version of the code has been merged to the “trunk” version of SAS4A. Software interfaces, inputs/outputs and physics modules have been well documented.

**Technology Transfer-Intellectual Property**
**Argonne National Laboratory background IP:**
SAS4A/SASSYS-1 liquid metal reactor accident analysis code

**Participant(s) background IP:**
Westinghouse Demonstration Lead-cooled Fast Reactor design
US Patent WO/2019/083695: "Pool Type Liquid Metal Fast Spectrum Reactor Using A Printed Circuit Heat Exchanger Connection To The Power Conversion System"

**Identify any new Subject Inventions as a result of this CRADA:**
Improvements to SAS4A/SASSYS-1 liquid metal reactor accident analysis code, DEFORM-4 MOX Fuel Performance Module

**Summary of technology transfer benefits to industry and, if applicable, path forward/anticipated next steps towards commercialization:**
The collaboration provides the computational capabilities to enable Westinghouse Electric Company to address LFR design and licensing challenges in support of its deployment as a promising new advanced reactor technology.

**Other information/results (papers, inventions, software, etc.):**
- Jun Liao *et.al.*, “Westinghouse Lead Fast Reactor Phenomena Identification and Ranking Table,” WCAP-18392-P, July 2019.
- Jun Liao *et.al.*, “The Importance of Phenomena Identification And Ranking Table In Lead Fast Reactor Development,” 18$^{th}$ International Meeting on Nuclear Reactor Thermal Hydraulics (NURETH-18), Portland, Oregon, USA, August 18-23, 2019.
- Moisseytsev, A., “CLFR SAS4A/SASSYS-1 Model,” ANL/NSE-19/45, November 18, 2019.
- Michael Epstein, “Blanketed Target Fuel Pin Temperature History,” Fauske & Associates, Intl. LLC report to Westinghouse Electric Company LLC, December 19, 2020.
- Michael Epstein, “Fuel/Heavy Liquid Metal Coolant Interaction Immediately After Fuel Pin Failure, Part I: Fission Gas Jet and Impingement Heat Transfer,” Fauske & Associates, Intl. LLC report to Westinghouse Electric Company LLC, September 9, 2020.
- Michael Epstein, “Fuel/Heavy Liquid Metal Coolant Interaction Immediately After Fuel Pin Failure, Part II: Fuel Expulsion from the Failed Fuel Pin,” Fauske & Associates, Intl. LLC report to Westinghouse Electric Company LLC, February 24, 2020.
- Michael Epstein, “Fuel/Heavy Liquid Metal Coolant Interaction Immediately After Fuel Pin Failure, Part III: The Interaction and Gas Blanketing Implications,” Fauske & Associates, Intl. LLC report to Westinghouse Electric Company LLC, March 31, 2020.

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